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Suppl. Mat. "Metallointercalators: Syntheses.....", Krotz, A. H. et al.

Table S1. Final Heavy Atom Parameters for [Rh(NH3)4phi]Cl3 x 3H2O

x, y, z and U_{eq}[a] $\times 10^4$

Atom	x	y	z	U_{eq}
Rh	3037(.3)	1649(.2)	3191(.1)	256
N1	1577(3)	282(3)	2754(1)	289(5)
C1	2374(4)	−480(3)	2122(2)	257(6)
C2	1609(4)	−1628(3)	1751(2)	281(6)
C3	−133(4)	−2024(4)	2099(2)	396(7)
C4	−819(4)	−3166(4)	1776(2)	470(8)
C5	214(5)	−3878(4)	1092(2)	470(8)
C6	1937(4)	−3487(3)	733(2)	403(7)
C7	2680(4)	−2366(3)	1059(2)	301(6)
C8	4551(4)	−1975(3)	695(2)	284(6)
C9	5612(4)	−2683(3)	−5(2)	380(7)
C10	7336(4)	−2313(4)	−344(2)	409(8)
C11	8065(4)	−1211(4)	−15(2)	403(8)
C12	7071(4)	−494(3)	678(2)	355(7)
C13	5319(4)	−870(3)	1037(2)	268(6)
C14	4271(4)	−131(3)	1777(2)	262(6)
N2	4795(3)	849(2)	2182(1)	273(5)
N3	4804(3)	2963(3)	3555(2)	364(6)
N4	1042(3)	2329(3)	4209(2)	408(6)
N5	2111(3)	3415(3)	2530(2)	364(6)

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Table S1 continued.

Atom	x	y	z	U_{eq}
N6	3941(3)	−96(3)	3860(2)	359(6)
Cl1	8495(1)	2335(1)	1988(1)	459(2)
Cl2	8036(1)	−86(1)	4180(1)	601(3)
Cl3	5726(2)	3399(1)	6911(1)	651(3)
W1	5468(3)	4533(3)	1468(2)	541(6)
W2	9657(6)	4417(4)	6049(3)	1243(14)
W3	3560(7)	3372(6)	5486(3)	1549(17)

[a] $U_{eq} = \frac{1}{3}\sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

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Table S2. Assigned Hydrogen Atom Parameters for [Rh(NH3)4phi]Cl3 x 3H2O

	x, y and $z \times 10^4$			
Atom	x	y	z	B
HN1	342	202	3009	2.6
H3	−874	−1487	2564	3.6
H4	−2023	−3435	2036	4.2
H5	−231	−4647	832	4.3
H6	2647	−3997	266	3.6
H9	5080	−3437	−236	3.4
H10	8047	−2805	−830	3.6
H11	9268	−977	−273	3.6
H12	7547	268	928	3.2
HN2	5967	1188	2018	2.4
HN3A	4502	3962	3403	3.3
HN3B	6005	2642	3271	3.3
HN3C	4673	2862	4124	3.3
HN4A	851	3374	4203	3.6
HN4B	1373	1962	4688	3.6
HN4C	−78	1929	4164	3.6
HN5A	1784	4240	2896	3.2
HN5B	1053	3148	2378	3.2
HN5C	3019	3612	2083	3.2
HN6A	5160	−11	3891	3.2
HN6B	3841	−1006	3625	3.2
HN6C	3195	−69	4418	3.2
HW1A	4707	4736	8125	4.9
HW1B	3468	5978	8363	4.9

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Table S3. Anisotropic Displacement Parameters for [Rh(NH3)4phi]Cl3 x 3H2O

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Rh	217(1)	296(1)	253(1)	−42(1)	−32(1)	−63(1)
N1	191(11)	362(13)	305(13)	−56(10)	−18(10)	−45(10)
C1	220(14)	287(14)	268(14)	−41(11)	−56(11)	−14(11)
C2	265(15)	290(14)	308(15)	−69(12)	−90(12)	−4(12)
C3	335(17)	457(18)	407(17)	−113(14)	−67(14)	−68(14)
C4	370(18)	485(20)	589(22)	−198(15)	−109(16)	−35(17)
C5	474(20)	388(18)	609(22)	−131(15)	−196(17)	−101(16)
C6	459(19)	342(16)	436(18)	−61(14)	−132(15)	−111(14)
C7	332(16)	267(14)	324(15)	−37(12)	−115(12)	3(12)
C8	310(15)	283(14)	266(14)	4(12)	−92(12)	−10(11)
C9	438(19)	366(17)	336(17)	−8(14)	−88(14)	−85(13)
C10	417(18)	449(18)	310(16)	49(14)	3(14)	−90(14)
C11	286(16)	487(19)	377(17)	−8(14)	45(13)	−39(14)
C12	309(16)	411(17)	330(16)	−59(13)	−22(13)	−70(13)
C13	255(14)	278(14)	258(14)	−12(11)	−34(11)	−18(11)
C14	232(14)	272(14)	282(14)	−28(11)	−57(11)	−1(11)
N2	211(12)	314(12)	289(12)	−78(9)	−18(9)	−55(10)
N3	353(14)	386(14)	373(14)	−83(11)	−93(11)	−85(11)
N4	353(14)	464(16)	377(14)	−16(12)	−13(12)	−120(12)
N5	373(14)	364(14)	375(14)	−20(11)	−124(11)	−48(11)
N6	382(14)	359(14)	334(14)	−28(11)	−75(11)	−36(11)
Cl1	276(4)	525(5)	587(5)	−95(3)	−93(4)	−11(4)
Cl2	409(5)	1033(8)	364(5)	−258(5)	−17(4)	10(5)
Cl3	848(7)	419(5)	739(7)	35(5)	−310(6)	−108(4)
W1	595(16)	499(14)	599(16)	−64(12)	−273(13)	−30(12)
W2	1531(38)	843(26)	1134(30)	165(25)	64(27)	−110(22)
W3	1881(47)	1723(44)	1242(36)	446(37)	−964(35)	−418(32)

$U_{i,j}$ values have been multiplied by 10^4

The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}\ell^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}h\ell a^*c^* + 2U_{23}k\ell b^*c^*)$$

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Table S4. Complete Distances and Angles for $[Rh(NH_3)_4phi]Cl_3 \times 3H_2O$

	Distance(Å)		Distance(Å)
Rh –N1	2.002(2)	N5 –HN5A	0.963
Rh –N2	2.010(2)	N5 –HN5B	0.952
Rh –N3	2.082(3)	N5 –HN5C	0.920
Rh –N4	2.075(3)	N6 –HN6A	0.951
Rh –N5	2.073(3)	N6 –HN6B	0.945
Rh –N6	2.061(2)	N6 –HN6C	0.975
N1 –C1	1.282(3)	W1 –HW1B	0.985
C1 –C2	1.461(4)	W1 –HW1A	0.947
C1 –C14	1.489(4)		
C2 –C3	1.397(4)		
C2 –C7	1.406(4)		
C3 –C4	1.383(5)		
C4 –C5	1.376(5)		
C5 –C6	1.387(5)		
C6 –C7	1.395(4)		
C7 –C8	1.487(4)		
C8 –C9	1.400(4)		
C8 –C13	1.408(4)		
C9 –C10	1.375(4)		
C10 –C11	1.377(4)		
C11 –C12	1.380(4)		
C12 –C13	1.401(4)		
C13 –C14	1.457(4)		
C14 –N2	1.283(3)		
N1 –HN1	0.948		
C3 –H3	0.967		
C4 –H4	0.971		
C5 –H5	0.962		
C6 –H6	0.950		
C9 –H9	0.962		
C10 –H10	0.965		
C11 –H11	0.959		
C12 –H12	0.960		
N2 –HN2	0.949		
N3 –HN3A	0.953		
N3 –HN3B	0.953		
N3 –HN3C	0.937		
N4 –HN4A	0.946		
N4 –HN4B	0.934		
N4 –HN4C	0.976		

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Table S4 continued.

			Angle(°)				Angle(°)
N1	-Rh	-N2	77.6(1)	N2	-C14	-C13	126.8(2)
N1	-Rh	-N3	173.7(1)	HN1	-N1	-C1	121.5
N1	-Rh	-N4	96.6(1)	H3	-C3	-C2	119.9
N1	-Rh	-N5	91.2(1)	H3	-C3	-C4	119.6
N1	-Rh	-N6	89.0(1)	H4	-C4	-C3	118.9
N2	-Rh	-N3	96.2(1)	H4	-C4	-C5	121.9
N2	-Rh	-N4	174.2(1)	H5	-C5	-C4	121.9
N2	-Rh	-N5	91.6(1)	H5	-C5	-C6	117.0
N2	-Rh	-N6	89.1(1)	H6	-C6	-C5	120.4
N3	-Rh	-N4	89.5(1)	H6	-C6	-C7	118.7
N3	-Rh	-N5	90.3(1)	H9	-C9	-C8	117.1
N3	-Rh	-N6	89.5(1)	H9	-C9	-C10	121.7
N4	-Rh	-N5	88.9(1)	H10	-C10	-C9	120.3
N4	-Rh	-N6	90.4(1)	H10	-C10	-C11	118.7
N5	-Rh	-N6	179.3(1)	H11	-C11	-C10	118.6
C2	-C1	-N1	126.3(2)	H11	-C11	-C12	121.8
C14	-C1	-N1	113.6(2)	H12	-C12	-C11	121.7
C14	-C1	-C2	120.0(2)	H12	-C12	-C13	118.2
C3	-C2	-C1	120.5(3)	HN2	-N2	-C14	121.8
C7	-C2	-C1	118.9(2)	Rh	-N3	-HN3A	107.9
C7	-C2	-C3	120.6(3)	Rh	-N3	-HN3B	108.0
C4	-C3	-C2	120.5(3)	Rh	-N3	-HN3C	108.8
C5	-C4	-C3	119.2(3)	Rh	-N4	-HN4A	109.3
C6	-C5	-C4	121.1(3)	Rh	-N4	-HN4B	109.9
C7	-C6	-C5	120.9(3)	Rh	-N4	-HN4C	107.8
C6	-C7	-C2	117.8(3)	Rh	-N5	-HN5A	106.8
C8	-C7	-C2	121.0(2)	Rh	-N5	-HN5B	107.3
C8	-C7	-C6	121.3(3)	Rh	-N5	-HN5C	108.9
C9	-C8	-C7	121.3(3)	Rh	-N6	-HN6A	110.2
C13	-C8	-C7	121.3(2)	Rh	-N6	-HN6B	110.4
C13	-C8	-C9	117.4(3)	Rh	-N6	-HN6C	109.0
C10	-C9	-C8	121.3(3)	HN3B	-N3	-HN3A	109.7
C11	-C10	-C9	121.0(3)	HN3C	-N3	-HN3A	111.1
C12	-C11	-C10	119.6(3)	HN3C	-N3	-HN3B	111.2
C13	-C12	-C11	120.1(3)	HN4B	-N4	-HN4A	112.1
C12	-C13	-C8	120.6(3)	HN4C	-N4	-HN4A	108.4
C14	-C13	-C8	119.0(2)	HN4C	-N4	-HN4B	109.3
C14	-C13	-C12	120.4(2)	HN5B	-N5	-HN5A	109.1
C13	-C14	-C1	119.7(2)	HN5C	-N5	-HN5A	111.7
N2	-C14	-C1	113.5(2)	HN5C	-N5	-HN5B	112.7

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Table S4 continued.

			Angle(°)
HN6B	-N6	-HN6A	110.6
HN6C	-N6	-HN6A	108.0
HN6C	-N6	-HN6B	108.5
HW1A	-W1	-HW1B	93.2

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Table S5. Interionic and Intermolecular Distances less than 3.5 Å for [Rh(NH3)4phi]Cl3 x 3H2O

	Distance(Å)		Distance(Å)
N1 -Cl1	3.309(2)	N5 -W2	3.117(5)
N1 -Cl2	3.204(2)	N5 -HW1A	3.056
C1 -Cl3	3.426(3)	N6 -Cl2	3.278(3)
C2 -H11	3.490	N6 -Cl2	3.286(3)
C3 -H12	3.441	N6 -Cl3	3.272(3)
C4 -C12	3.477(4)	Cl1 -W1	3.151(3)
C4 -HW1B	3.448	Cl1 -H12	2.875
C4 -HW1A	3.374	Cl1 -HN2	2.263
C5 -C11	3.499(5)	Cl1 -HN3B	2.524
C5 -HN5B	3.493	Cl1 -HW1B	2.193
C5 -HW1B	3.474	Cl1 -H5	3.388
C5 -H10	3.174	Cl1 -HN1	2.994
C6 -H9	3.423	Cl1 -HN5B	2.375
C6 -H10	3.364	Cl1 -H10	2.951
C7 -HW1A	3.261	Cl1 -H11	3.207
C8 -W1	3.449(4)	Cl1 -HW1A	3.457
C8 -C12	3.494(4)	Cl2 -HN3B	3.299
C8 -HW1A	3.221	Cl2 -HN6A	2.339
C9 -W1	3.458(4)	Cl2 -HN1	2.340
C9 -H6	3.177	Cl2 -H3	2.939
C9 -W1	3.311(4)	Cl2 -HN4C	2.428
C10 -H5	3.362	Cl2 -W3	3.312(5)
C10 -H6	3.348	Cl2 -HN4B	2.588
C10 -HN5B	3.430	Cl2 -HN6C	2.325
C10 -HN5C	3.254	Cl3 -W2	3.220(4)
C11 -H11	3.097	Cl3 -W3	3.192(5)
C12 -H11	3.131	Cl3 -HW1A	2.341
N2 -HW1B	3.299	Cl3 -H4	2.962
N3 -Cl1	3.397(3)	Cl3 -HN6B	2.345
N3 -W3	3.179(6)	Cl3 -W1	3.259(3)
N3 -Cl3	3.374(3)	Cl3 -HN3A	2.434
N3 -HW1A	3.415	Cl3 -HN5A	3.066
N4 -W3	3.389(6)	Cl3 -HW1B	3.474
N4 -Cl2	3.327(3)	W1 -HN2	3.154
N4 -Cl2	3.478(3)	W1 -HN3A	3.188
N4 -W2	2.984(5)	W1 -HN5A	3.271
N5 -W1	3.004(3)	W1 -HN5C	2.145
N5 -HW1B	3.445	W1 -H4	3.096
N5 -Cl1	3.326(3)	W1 -H5	3.351
N5 -H10	2.948	W1 -H6	3.411

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Table S5 continued.

		Distance(Å)			Distance(Å)
W1	-H9	3.392	HN3A	-HW1A	2.742
W1	-H6	2.964	HN3B	-HW1B	2.925
W1	-H9	2.456	HN3B	-HW1A	3.367
W2	-W3	2.974(6)	HN5A	-HW1A	3.035
W2	-HN4A	3.167	HN5C	-HW1B	2.665
W2	-HN4B	3.211	HN5C	-HW1A	2.358
W2	-HN3A	3.300			
W2	-HN4A	2.053			
W2	-HN4C	3.363			
W2	-HN5A	2.196			
W2	-HN5B	3.413			
W3	-HN3A	3.429			
W3	-HN3C	2.291			
W3	-HN4A	3.295			
W3	-HN4B	2.781			
W3	-HN6A	3.317			
W3	-HN6B	3.319			
H3	-HN2	3.494			
H3	-HN6A	3.495			
H4	-HW1B	2.815			
H4	-HW1A	2.525			
H5	-HN5B	3.470			
H5	-HW1B	2.880			
H5	-H5	2.815			
H5	-H6	3.224			
H5	-H10	2.714			
H5	-HW1A	3.463			
H6	-H9	2.758			
H6	-H10	3.079			
H9	-H10	2.367			
H9	-HW1A	3.335			
H9	-H9	2.926			
H9	-HN5C	3.104			
H9	-HW1B	2.967			
H10	-HN5B	2.547			
H10	-HN5C	2.567			
H11	-H11	2.487			
H11	-H12	2.557			
HN2	-HW1B	2.681			
HN3A	-HW1B	3.008			

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Table S6. Final Heavy Atom Parameters for [Rh([12]aneN4)phi](SCN)3 x 2H2O

x, y, z and U_{eq}[a] $\times 10^4$

Atom	x	y	z	U_{eq} or B	
Rh	7273(.4)	2226(.6)	3329(.8)	333(2)	
N1	7680(4)	3493(5)	3775(7)	341(16)	
C1	8444(5)	3638(6)	3179(9)	304(20)	
C2	8819(5)	4550(7)	3279(9)	352(21)	
C3	8332(6)	5426(8)	4025(10)	486(25)	
C4	8676(7)	6300(8)	4096(11)	599(29)	
C5	9519(8)	6322(8)	3407(11)	600(29)	
C6	10007(6)	5475(8)	2679(10)	513(24)	
C7	9675(5)	4570(7)	2598(9)	402(23)	
C8	10198(5)	3635(7)	1832(9)	385(23)	
C9	11098(6)	3554(9)	1286(11)	596(28)	
C10	11584(6)	2700(10)	577(11)	632(32)	
C11	11212(6)	1882(8)	385(10)	540(28)	
C12	10338(6)	1913(7)	899(9)	434(24)	
C13	9825(5)	2791(7)	1626(9)	346(21)	
C14	8913(5)	2813(7)	2229(8)	299(20)	
N2	8457(4)	2147(5)	2065(7)	342(16)	
N3	7004(4)	938(6)	2636(8)	459(17)	
C15A	7726(7)	−143(10)	3215(13)	4.6(3)	*
C15B	7107	−274	3954	4.4	*

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Table S6 continued.

Atom	x	y	z	U_{eq} or B	
C16	7906(6)	−352(7)	4949(11)	596(29)	
N4	7845(4)	805(6)	5304(7)	417(18)	
C17	7225(6)	977(8)	6718(10)	523(25)	
C18	6247(6)	1465(8)	6184(10)	520(26)	
N5	6173(4)	2522(5)	4795(7)	369(17)	
C19	5317(5)	3088(8)	3845(11)	560(27)	
C20	5518(6)	3968(8)	2328(11)	661(31)	
N6	6352(4)	3346(6)	1527(8)	475(19)	
C21	6152(7)	2611(9)	589(11)	710(29)	
C22A	6782(7)	1405(10)	948(13)	4.3(3)	*
C22B	6168	1354	1603	4.4	*
S1	9729(2)	1008(2)	6385(4)	710(8)	
C23	9205(7)	1107(8)	8108(17)	786(39)	
N7	8838(7)	1162(10)	9311(13)	732(31)	
S2	7086(2)	5165(3)	8452(3)	916(9)	
C24	6770(6)	4585(8)	7217(11)	562(28)	
N8	6496(5)	4205(7)	6357(10)	673(23)	
S3	3861(3)	3319(4)	8373(6)	1090(14)	
C25	3753	2591	7160	8.6	*
N9	3688(10)	2022(14)	6410(26)	1853(72)	

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Table S6 continued.

Atom	x	y	z	U_{eq} or B	
S4A	3874	2518	8150	8.0	*
C26A	4097	1302	9640	9.0	*
N10A	4261	438	10744	8.9	*
S4B	4261	438	10744	8.0	*
C26B	4030	1668	9192	9.0	*
N10B	3874	2518	8150	8.9	*
O1	5344(7)	274(10)	3459(15)	1853(41)	
O2	3638(9)	1807(13)	3104(22)	3174(77)	

[a] $U_{eq} = \frac{1}{3}\sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

* Isotropic displacement parameter, B

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Table S7. Assigned Hydrogen Atom Parameters for [Rh([12]aneN4)phi](SCN)3 x 2H2O

x, y and $z \times 10^4$

Atom	x	y	z	B
HN1	7312	3971	4427	3.1
H3	7758	5414	4520	4.4
H4	8334	6886	4595	5.5
H5	9761	6935	3443	5.4
H6	10572	5525	2234	4.6
H9	11363	4108	1415	5.5
H10	12184	2685	208	5.8
H11	11566	1304	−120	4.9
H12	10085	1335	746	4.0
HN2	8667	1643	1381	3.1
HN3A	6477	731	3115	4.2
HN3B	7507	769	1939	4.2
HN4	8443	765	5517	3.8
HN5	6151	3105	5308	3.3
HN6	6585	3931	782	4.3
H15A	8253	−94	2603	5.3
H15B	7542	−790	3128	5.3
H15C	7256	−915	3486	5.3
H15D	6569	−269	4593	5.3
H16A	8501	−887	5205	5.3
H16B	7473	−691	5613	5.3
H16C	8456	−574	4372	5.3
H16D	7921	−947	5959	5.3
H17A	7372	1519	7151	4.8
H17B	7318	226	7532	4.8
H18A	5859	1685	7034	4.7
H18B	6073	885	5883	4.7
H19A	4846	3497	4441	5.1
H19B	5132	2504	3576	5.1
H20A	5630	4596	2605	6.0
H20B	5022	4266	1622	6.0

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Table S8 continued.

Atom	*x*	*y*	*z*	*B*
H21A	6196	3023	−533	6.3
H21B	5553	2581	841	6.3
H21C	6598	2570	−251	6.3
H21D	5567	3037	125	6.3
H22A	7335	1419	333	4.9
H22B	6518	903	660	4.9
H22C	6225	854	931	4.9
H22D	5632	1364	2251	4.9

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Table S9. Anisotropic Displacement Parameters for [Rh([12]aneN$_4$)phi](SCN)$_3$ x 2H$_2$O

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Rh	327(4)	351(4)	349(4)	−116(3)	−5(3)	−126(3)
N1	287(39)	366(41)	449(42)	−87(32)	26(33)	−251(34)
C1	286(49)	291(49)	328(48)	−59(40)	−90(39)	−80(40)
C2	438(54)	293(51)	345(49)	−181(44)	−63(41)	−28(41)
C3	635(60)	340(54)	466(56)	−161(49)	−31(46)	−69(46)
C4	874(78)	353(59)	667(68)	−272(55)	−134(58)	−153(50)
C5	900(80)	428(64)	556(64)	−383(60)	−239(58)	3(52)
C6	630(62)	457(60)	512(60)	−338(54)	−137(48)	−2(50)
C7	473(57)	394(56)	325(50)	−200(47)	−100(43)	18(43)
C8	374(55)	445(56)	285(48)	−171(45)	−51(40)	32(42)
C9	480(65)	754(74)	549(63)	−306(56)	−21(51)	−51(57)
C10	355(57)	828(79)	606(68)	−163(59)	71(49)	−96(61)
C11	424(62)	632(68)	442(58)	−37(51)	39(46)	−124(50)
C12	371(55)	489(58)	371(51)	−86(45)	−10(42)	−66(46)
C13	331(51)	425(54)	272(47)	−138(45)	−35(39)	−50(42)
C14	326(50)	334(50)	255(46)	−136(42)	−39(38)	−63(40)
N2	363(39)	410(42)	294(39)	−138(35)	69(30)	−159(33)
N3	545(45)	467(46)	462(45)	−244(38)	−78(35)	−154(37)
C16	557(59)	366(57)	767(72)	−76(45)	23(50)	−101(51)
N4	326(39)	439(45)	437(44)	−71(33)	−75(33)	−80(35)
C17	545(60)	594(61)	392(55)	−161(48)	−22(47)	−95(46)
C18	508(59)	609(64)	379(55)	−161(48)	37(44)	−74(50)
N5	325(40)	407(43)	370(42)	−90(33)	45(32)	−141(36)
C19	398(55)	591(63)	562(62)	−64(47)	26(47)	−84(52)
C20	384(56)	671(68)	702(71)	−34(50)	−76(50)	12(58)
N6	440(45)	520(46)	412(43)	−173(37)	−15(35)	−29(37)
C21	827(72)	1007(85)	451(59)	−516(67)	−124(52)	−144(58)
S1	603(17)	705(19)	893(21)	−212(14)	−147(15)	−272(16)
C23	566(72)	380(61)	1566(124)	192(52)	−706(78)	−619(80)
N7	566(69)	922(86)	831(84)	185(57)	−211(58)	−785(75)
S2	1113(24)	1266(27)	683(19)	−850(22)	24(17)	−226(18)

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Table S9 continued.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C24	557(62)	630(67)	425(61)	−184(51)	127(48)	−88(52)
N8	753(58)	761(61)	598(57)	−217(46)	194(45)	−404(49)
S3	987(30)	882(30)	1467(41)	−461(25)	−232(28)	−175(28)
N9	1076(114)	1376(140)	3360(255)	−452(101)	597(136)	−1157(160)
O1	1616(92)	2125(113)	2533(128)	−1264(87)	479(87)	−1117(103)
O2	2210(133)	2410(151)	4341(244)	−1562(120)	−1610(149)	1223(153)

$U_{i,j}$ values have been multiplied by 10^4

The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}\ell^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}h\ell a^*c^* + 2U_{23}k\ell b^*c^*)$$

Table S10. Complete Distances and Angles for [Rh([12]aneN4)phi](SCN)3 x 2H2O

		Distance(Å)			Distance(Å)
Rh	-N1	2.007(6)	C18	-N5	1.460(11)
Rh	-N2	2.026(6)	N5	-C19	1.487(11)
Rh	-N3	2.026(7)	C19	-C20	1.502(13)
Rh	-N4	2.068(6)	C20	-N6	1.499(12)
Rh	-N5	2.021(6)	N6	-C21	1.505(12)
Rh	-N6	2.067(7)	C21	-C22A	1.454(15)
N1	-C1	1.283(10)	C21	-C22B	1.521(18)
C1	-C2	1.445(11)	S1	-C23	1.644(12)
C1	-C14	1.470(11)	C23	-N7	1.146(16)
C2	-C3	1.401(12)	S2	-C24	1.643(10)
C2	-C7	1.398(11)	C24	-N8	1.168(13)
C3	-C4	1.363(13)	S3	-C25	1.628(15)
C4	-C5	1.381(14)	C25	-N9	1.124(18)
C5	-C6	1.365(14)	S4A	-C26A	1.615
C6	-C7	1.390(12)	C26A	-N10A	1.169
C7	-C8	1.479(12)	S4B	-C26B	1.655
C8	-C9	1.406(13)	C26B	-N10B	1.129
C8	-C13	1.401(11)	N1	-HN1	0.957
C9	-C10	1.360(14)	C3	-H3	0.947
C10	-C11	1.366(14)	C4	-H4	0.943
C11	-C12	1.372(13)	C5	-H5	0.951
C12	-C13	1.402(12)	C6	-H6	0.931
C13	-C14	1.447(11)	C9	-H9	0.939
C14	-N2	1.286(10)	C10	-H10	0.947
N3	-C15A	1.427(13)	C11	-H11	0.944
N3	-C15B	1.549(18)	C12	-H12	0.962
C15A	-C15B	1.124(18)	N2	-HN2	0.950
N3	-C22A	1.434(13)	N3	-HN3A	0.949
N3	-C22B	1.511(18)	N3	-HN3B	0.944
C22A	-C22B	1.066(18)	C15A	-H15A	0.934
C15A	-C16	1.487(15)	C15A	-H15B	0.952
C15B	-C16	1.54(18)	C15B	-H15C	0.950
C16	-N4	1.520(11)	C15B	-H15D	0.950
N4	-C17	1.503(11)	C16	-H16A	0.950
C17	-C18	1.505(12)	C16	-H16B	0.950

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Table S10 continued.

		Distance(Å)				Angle(°)
C16	-H16C	0.947	N1	-Rh	-N2	76.8(3)
C16	-H16D	0.951	N1	-Rh	-N3	171.8(3)
N4	-HN4	0.946	N1	-Rh	-N4	99.1(3)
C17	-H17A	0.952	N1	-Rh	-N5	91.6(3)
C17	-H17B	0.954	N1	-Rh	-N6	97.3(3)
C18	-H18A	0.952	N2	-Rh	-N3	95.2(3)
C18	-H18B	0.950	N2	-Rh	-N4	95.0(2)
N5	-HN5	0.945	N2	-Rh	-N5	168.1(2)
C19	-H19A	0.949	N2	-Rh	-N6	100.2(3)
C19	-H19B	0.949	N3	-Rh	-N4	82.9(3)
C20	-H20A	0.947	N3	-Rh	-N5	96.5(3)
C20	-H20B	0.939	N3	-Rh	-N6	82.5(3)
C21	-H21A	0.956	N4	-Rh	-N5	84.5(3)
C21	-H21B	0.940	N4	-Rh	-N6	159.8(3)
C21	-H21C	0.951	N5	-Rh	-N6	83.4(3)
C21	-H21D	0.950	Rh	-N1	-C1	118.6(5)
C22A	-H22A	0.962	Rh	-N2	-C14	116.9(5)
C22A	-H22B	0.942	Rh	-N3	-C15A	107.4(6)
C22B	-H22C	0.950	Rh	-N3	-C22A	108.1(6)
C22B	-H22D	0.950	Rh	-N3	-C15B	116.2
N6	-HN6	0.946	Rh	-N3	-C22B	115.3
O1	-H22D	1.586	Rh	-N4	-C16	108.5(5)
			Rh	-N4	-C17	106.2(5)
			Rh	-N5	-C18	109.9(5)
			Rh	-N5	-C19	111.1(5)
			Rh	-N6	-C20	107.5(5)
			Rh	-N6	-C21	108.8(5)
			C2	-C1	-N1	126.4(7)
			C14	-C1	-N1	113.1(7)
			C14	-C1	-C2	120.4(7)
			C3	-C2	-C1	121.1(7)
			C7	-C2	-C1	119.5(7)
			C7	-C2	-C3	119.4(7)
			C4	-C3	-C2	121.3(8)
			C5	-C4	-C3	119.1(9)

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Table S10 continued.

			Angle(°)				Angle(°)
C6	-C5	-C4	120.7(9)	N7	-C23	-S1	179.1(11)
C7	-C6	-C5	121.4(9)	N8	-C24	-S2	176.2(9)
C6	-C7	-C2	118.1(8)	N9	-C25	-S3	175.4
C8	-C7	-C2	119.6(7)	N10A	-C26A	-S4A	178.3
C8	-C7	-C6	122.3(8)	N10B	-C26B	-S4B	178.8
C9	-C8	-C7	121.1(8)	Rh	-N1	-HN1	120.3
C13	-C8	-C7	121.8(7)	Rh	-N2	-HN2	121.8
C13	-C8	-C9	117.1(8)	Rh	-N3	-HN3A	115.1
C10	-C9	-C8	121.6(9)	Rh	-N3	-HN3B	99.5
C11	-C10	-C9	120.7(9)	Rh	-N4	-HN4	112.7
C12	-C11	-C10	120.4(9)	Rh	-N5	-HN5	112.8
C13	-C12	-C11	119.7(8)	Rh	-N6	-HN6	112.3
C12	-C13	-C8	120.5(7)	HN1	-N1	-C1	121.1
C14	-C13	-C8	118.8(7)	H3	-C3	-C2	120.7
C14	-C13	-C12	120.6(7)	H3	-C3	-C4	118.0
C13	-C14	-C1	119.0(7)	H4	-C4	-C3	119.9
N2	-C14	-C1	114.3(7)	H4	-C4	-C5	121.1
N2	-C14	-C13	126.6(7)	H5	-C5	-C4	119.5
C22A	-N3	-C15A	120.5(8)	H5	-C5	-C6	119.7
C22B	-N3	-C15B	113.6(14)	H6	-C6	-C5	117.7
C16	-C15A	-N3	110.3(9)	H6	-C6	-C7	120.9
C16	-C15B	-N3	101.3(14)	H9	-C9	-C8	118.6
N4	-C16	-C15A	111.6(8)	H9	-C9	-C10	119.8
N4	-C16	-C15B	114.6(16)	H10	-C10	-C9	119.0
C17	-N4	-C16	111.7(6)	H10	-C10	-C11	120.4
C18	-C17	-N4	110.0(7)	H11	-C11	-C10	118.6
N5	-C18	-C17	107.4(7)	H11	-C11	-C12	121.0
C19	-N5	-C18	119.5(6)	H12	-C12	-C11	119.3
C20	-C19	-N5	106.7(7)	H12	-C12	-C13	121.0
N6	-C20	-C19	109.0(7)	HN2	-N2	-C14	121.3
C21	-N6	-C20	112.4(7)	HN3A	-N3	-C15A	103.4
C22A	-C21	-N6	112.7(8)	HN3A	-N3	-C22A	102.6
C22B	-C21	-N6	114.1(17)	HN3B	-N3	-C15B	103.8
C21	-C22A	-N3	110.9(9)	HN3B	-N3	-C22B	105.9
C21	-C22B	-N3	103.3(15)	H15A	-C15A	-N3	109.7

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Table S10 continued.

			Angle(°)				Angle(°)
H15B	-C15A	-N3	108.2	H20A	-C20	-N6	109.0
H15A	-C15A	-C16	109.6	H20B	-C20	-N6	109.6
H15B	-C15A	-C16	108.3	H20B	-C20	-H20A	110.7
H15B	-C15A	-H15A	110.7	HN6	-N6	-C20	108.8
H16A	-C16	-C15A	108.9	HN6	-N6	-C21	107.2
H16B	-C16	-C15A	109.8	H21A	-C21	-N6	106.7
H16A	-C16	-N4	108.5	H21B	-C21	-N6	107.8
H16B	-C16	-N4	108.5	H21C	-C21	-N6	106.7
H16C	-C16	-N4	107.9	H21D	-C21	-N6	106.8
H16D	-C16	-N4	107.6	H21A	-C21	-C22A	109.8
H16C	-C16	-C15B	108.7	H21B	-C21	-C22A	110.1
H16D	-C16	-C15B	108.4	H21C	-C21	-C22B	109.9
H16B	-C16	-H16A	109.5	H21D	-C21	-C22B	109.9
H16D	-C16	-H16C	109.6	H21B	-C21	-H21A	109.8
HN4	-N4	-C16	107.1	H21D	-C21	-H21C	109.4
HN4	-N4	-C17	110.7	H22A	-C22A	-N3	108.5
H17A	-C17	-N4	108.9	H22B	-C22A	-N3	109.4
H17B	-C17	-N4	109.1	H22A	-C22A	-C21	109.4
H17A	-C17	-C18	110.1	H22B	-C22A	-C21	109.5
H17B	-C17	-C18	109.8	H22B	-C22A	-H22A	109.1
H17B	-C17	-H17A	108.9	H15C	-C15B	-N3	111.1
H18A	-C18	-C17	110.3	H15D	-C15B	-N3	111.7
H18B	-C18	-C17	110.4	H15C	-C15B	-C16	111.4
H18A	-C18	-N5	109.5	H15D	-C15B	-C16	111.7
H18B	-C18	-N5	109.9	H15D	-C15B	-H15C	109.5
H18B	-C18	-H18A	109.3	H22C	-C22B	-N3	110.7
HN5	-N5	-C18	101.4	H22D	-C22B	-N3	111.3
HN5	-N5	-C19	101.3	H22C	-C22B	-C21	110.7
H19A	-C19	-N5	110.4	H22D	-C22B	-C21	111.2
H19B	-C19	-N5	110.7	H22D	-C22B	-H22C	109.5
H19A	-C19	-C20	109.6				
H19B	-C19	-C20	109.8				
H19B	-C19	-H19A	109.7				
H20A	-C20	-C19	109.0				
H20B	-C20	-C19	109.5				

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Table S1Ω. Interionic and Intermolecular Distances less than 3.5 Å for [Rh([12]aneN$_4$)phi](SCN)$_3$ x 2H$_2$O

		Distance(Å)
C3	–C25	3.405
C4	–C6	3.374(13)
C5	–C11	3.424(14)
C5	–C6	3.442(14)
C12	–N7	3.312(14)
C12	–C23	3.400(14)
N2	–N7	2.927(13)
N3	–O1	2.893(14)
C15B	–O1	2.643
C15B	–N9	2.902
C15B	–O2	3.035
C16	–O2	3.432(19)
N4	–S1	3.261(7)
C18	–N10A	3.178
C18	–S4B	3.178
N5	–N8	2.984(10)
C19	–N9	3.49(2)
C20	–C24	3.466(13)
N6	–S2	3.276(7)
C21	–C24	3.450(14)
C22A	–O1	3.275(16)
C22A	–N7	3.307(16)
C22B	–O1	2.305
S2	–O2	3.399(17)
N9	–O2	2.97(2)
N9	–O1	2.72(2)
O1	–O2	2.70(2)
O1	–N10A	2.954
O1	–S4B	2.954
O1	–O1	2.738(17)
O1	–O2	3.42(2)
O2	–C26A	3.217
O2	–N10A	2.940
O2	–S4B	2.940
O2	–C26B	3.432

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Table S10. Final Heavy Atom Parameters of [Rh([12]aneS4)phi]Br3 x 3H2O

x, y, z and $U_{eq}{}^{a} \times 10^{4}$

Atom	x	y	z	U_{eq}
Rh	8720(.8)	2518(.6)	3302(.6)	222(2)
N1	10314(8)	1785(6)	2580(6)	262(21)
C1	9908(10)	989(7)	2282(7)	218(26)
C2	10903(10)	394(7)	1728(7)	236(25)
C3	12374(10)	733(8)	1400(7)	335(28)
C4	13293(11)	169(9)	873(8)	437(32)
C5	12767(12)	−720(9)	664(8)	448(31)
C6	11[illegible]3(12)	−1040(8)	966(8)	419(29)
C7	10355(10)	−508(8)	1506(7)	272(27)
C8	8801(10)	−834(8)	1811(7)	266(25)
C9	8240(12)	−1729(8)	1571(8)	399(29)
C10	6778(12)	−2041(8)	1855(8)	406(29)
C11	5826(11)	−1467(8)	2366(8)	352(27)
C12	6332(11)	−604(8)	2619(7)	331(26)
C13	7808(10)	−269(7)	2337(7)	237(25)
C14	8344(10)	665(7)	2594(7)	238(30)
N2	7581(8)	1268(6)	3072(6)	243(20)
S1	9268(3)	1446(2)	5079(2)	309(6)
C15	10521(10)	2366(8)	5403(7)	356(28)
C16	10210(11)	3575(8)	4846(7)	325(27)

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Table S18 continued.

Atom	x	y	z	U_{eq}
S2	10381(3)	3760(2)	3428(2)	296(6)
C17	9449(11)	5059(8)	2745(8)	376(28)
C18	9092(10)	5022(8)	1654(8)	364(30)
S3	8011(3)	3854(2)	1689(2)	305(7)
C19	6121(10)	4327(8)	2028(7)	345(27)
C20	5410(10)	3510(8)	3018(8)	331(27)
S4	6732(3)	3267(2)	4054(2)	267(6)
C21	6204(10)	2038(8)	5144(7)	301(25)
C22	7521(11)	1655(8)	5833(7)	331(26)
Br1	6828(1)	4053(1)	6663(1)	476(3)
Br2	7383(1)	6230(1)	−813(1)	503(3)
Br3	6673(1)	−1000(1)	5983(1)	471(3)
W1	5821(8)	2247(6)	985(6)	585(21)
W2	3417(8)	3992(6)	5701(6)	697(25)
W3	7466(9)	3621(7)	9187(6)	734(25)

[a] $U_{eq} = \frac{1}{3}\sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

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Table S14. Assigned Hydrogen Atom Parameters of [Rh([12]aneS4)phi]Br3 x 3H2O

x, y and $z \times 10^4$

Atom	x	y	z	B
HN1	11325	2019	2467	2.4
H3	12737	1348	1545	2.9
H4	14287	397	647	3.9
H5	13423	−1116	315	4.0
H6	10969	−1642	789	3.7
H9	8872	−2129	1218	3.6
H10	6426	−2646	1697	3.7
H11	4816	−1672	2540	3.2
H12	5673	−234	2991	2.9
HN2	6561	1143	3303	2.2
H15A	11518	2189	5214	3.2
H15B	10415	2232	6148	3.2
H16A	10915	3996	5025	2.9
H16B	9219	3785	5035	2.9
H17A	10084	5648	2670	3.3
H17B	8544	5150	3129	3.3
H18A	10017	4993	1268	3.2
H18B	8538	5683	1296	3.2
H19A	5503	4427	1447	3.1
H19B	6200	5012	2144	3.1
H20A	5243	2842	2896	3.0
H20B	4489	3814	3212	3.0
H21A	5956	1480	4870	2.7
H21B	5369	2210	5544	2.7
H22A	7289	971	6367	3.0
H22B	7683	2189	6158	3.0

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Table S13. Anisotropic Displacement Parameters of [Rh([12]aneS4)phi]Br3 x 3H2O

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Rh	192(5)	293(5)	209(5)	−1(4)	7(4)	−124(4)
N1	164(46)	364(52)	304(49)	1(39)	31(38)	−183(44)
C1	301(68)	225(59)	134(53)	−56(49)	−23(47)	−57(48)
C2	248(65)	264(62)	199(57)	48(50)	55(48)	−100(50)
C3	245(66)	413(68)	338(63)	2(54)	69(53)	−129(56)
C4	256(64)	668(86)	437(71)	51(61)	127(55)	−288(67)
C5	393(80)	554(81)	491(75)	42(62)	130(60)	−336(66)
C6	379(76)	538(77)	439(72)	9(61)	22(59)	−306(64)
C7	290(66)	351(67)	178(56)	75(53)	−6(49)	−108(52)
C8	241(63)	318(65)	253(59)	53(52)	−55(50)	−116(52)
C9	528(81)	389(71)	349(67)	−45(61)	36(58)	−219(58)
C10	476(79)	356(69)	421(71)	−108(60)	11(60)	−165(59)
C11	290(64)	437(71)	345(65)	−157(57)	73(53)	−142(58)
C12	338(72)	395(70)	325(64)	−65(56)	48(53)	−208(56)
C13	290(66)	251(61)	180(56)	−15(52)	−11(49)	−85(50)
C14	235(63)	294(63)	116(53)	48(52)	−2(46)	13(49)
N2	166(44)	352(51)	229(46)	12(39)	59(36)	−134(42)
S1	343(16)	310(16)	275(15)	18(13)	−20(13)	−103(13)
C15	308(64)	485(76)	301(62)	−45(54)	−36(50)	−155(58)
C16	409(65)	424(71)	200(57)	−51(53)	−25(49)	−172(54)
S2	273(15)	356(17)	286(15)	−20(12)	−11(12)	−139(13)
C17	454(70)	297(65)	389(69)	−81(53)	−12(55)	−120(55)
C18	232(60)	507(72)	306(64)	−25(51)	30(49)	−78(55)
S3	310(16)	392(17)	222(14)	−34(13)	2(12)	−111(13)
C19	306(63)	414(67)	315(64)	15(52)	−58(51)	−116(55)
C20	211(58)	374(65)	422(67)	58(49)	−44(51)	−155(56)
S4	232(14)	336(16)	258(15)	0(12)	45(12)	−142(13)
C21	236(59)	388(65)	301(61)	−35(50)	24(50)	−147(52)
C22	369(65)	412(67)	241(59)	−164(52)	127(52)	−147(52)
Br1	517(8)	553(8)	456(7)	−23(6)	−48(6)	−291(6)
Br2	426(8)	569(8)	435(7)	10(6)	−33(6)	−62(6)

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Table S13 continued

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br3	382(7)	454(8)	624(8)	−24(6)	−144(6)	−219(6)
W1	572(52)	565(52)	651(53)	−8(41)	−14(43)	−252(44)
W2	517(52)	656(57)	830(61)	−73(43)	−100(46)	−109(49)
W3	956(67)	819(61)	468(51)	−278(51)	26(47)	−240(47)

$U_{i,j}$ values have been multiplied by 10^4

The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}\ell^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}h\ell a^*c^* + 2U_{23}k\ell b^*c^*)$$

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Table S14. Complete Distances and Angles of [Rh([12]aneS4)phi]Br3 x 3H2O

	Distance(Å)		Distance(Å)
Rh –N1	2.029(7)	C6 –H6	0.955
Rh –N2	2.065(7)	C9 –H9	0.948
Rh –S1	2.373(3)	C10 –H10	0.946
Rh –S2	2.292(3)	C11 –H11	0.946
Rh –S3	2.355(3)	C12 –H12	0.952
Rh –S4	2.302(3)	N2 –HN2	0.947
S1 –C15	1.840(10)	C15 –H15A	0.946
S1 –C22	1.856(10)	C15 –H15B	0.948
S2 –C16	1.822(10)	C16 –H16A	0.944
S2 –C17	1.795(10)	C16 –H16B	0.952
S3 –C18	1.816(10)	C17 –H17A	0.946
S3 –C19	1.839(10)	C17 –H17B	0.951
S4 –C20	1.808(10)	C18 –H18A	0.951
S4 –C21	1.815(10)	C18 –H18B	0.950
N1 –C1	1.291(12)	C19 –H19A	0.948
C1 –C2	1.461(13)	C19 –H19B	0.951
C1 –C14	1.474(13)	C20 –H20A	0.946
C2 –C3	1.404(13)	C20 –H20B	0.948
C2 –C7	1.407(13)	C21 –H21A	0.948
C3 –C4	1.374(15)	C21 –H21B	0.947
C4 –C5	1.375(16)	C22 –H22A	0.952
C5 –C6	1.370(15)	C22 –H22B	0.946
C6 –C7	1.384(14)		
C7 –C8	1.465(13)		
C8 –C9	1.416(14)		
C8 –C13	1.411(13)		
C9 –C10	1.379(15)		
C10 –C11	1.385(15)		
C11 –C12	1.369(14)		
C12 –C13	1.399(13)		
C13 –C14	1.465(13)		
C14 –N2	1.297(12)		
C15 –C16	1.498(14)		
C17 –C18	1.524(14)		
C19 –C20	1.514(14)		
C21 –C22	1.494(13)		
N1 –HN1	0.954		
C3 –H3	0.951		
C4 –H4	0.950		
C5 –H5	0.952		

Table S14 continued.

	Angle(°)		Angle(°)
N1 -Rh -N2	77.2(3)	C13 -C8 -C9	117.7(9)
N1 -Rh -S1	96.5(2)	C10 -C9 -C8	120.9(10)
N1 -Rh -S2	91.8(2)	C11 -C10 -C9	120.2(10)
N1 -Rh -S3	93.6(2)	C12 -C11 -C10	120.5(9)
N1 -Rh -S4	174.1(2)	C13 -C12 -C11	120.4(9)
N2 -Rh -S1	93.1(2)	C12 -C13 -C8	120.3(8)
N2 -Rh -S2	168.9(2)	C14 -C13 -C8	119.4(8)
N2 -Rh -S3	94.4(2)	C14 -C13 -C12	120.4(8)
N2 -Rh -S4	97.3(2)	C13 -C14 -C1	118.5(8)
S1 -Rh -S2	87.3(1)	N2 -C14 -C1	114.5(8)
S1 -Rh -S3	168.5(1)	N2 -C14 -C13	127.0(8)
S1 -Rh -S4	85.6(1)	Rh -N1 -HN1	121.2
S2 -Rh -S3	87.1(1)	HN1 -N1 -C1	121.4
S2 -Rh -S4	93.8(1)	H3 -C3 -C2	120.2
S3 -Rh -S4	84.8(1)	H3 -C3 -C4	120.1
Rh -N1 -C1	117.4(6)	H4 -C4 -C3	120.0
Rh -N2 -C14	116.1(6)	H4 -C4 -C5	120.0
Rh -S1 -C15	100.5(3)	H5 -C5 -C4	119.2
Rh -S1 -C22	102.2(3)	H5 -C5 -C6	120.4
Rh -S2 -C16	101.6(3)	H6 -C6 -C5	119.1
Rh -S2 -C17	102.1(3)	H6 -C6 -C7	119.0
Rh -S3 -C18	101.8(3)	H9 -C9 -C8	120.2
Rh -S3 -C19	103.1(3)	H9 -C9 -C10	118.9
Rh -S4 -C20	99.0(3)	H10 -C10 -C9	119.8
Rh -S4 -C21	99.0(3)	H10 -C10 -C11	120.0
C2 -C1 -N1	124.4(8)	H11 -C11 -C10	119.8
C14 -C1 -N1	114.7(8)	H11 -C11 -C12	119.6
C14 -C1 -C2	120.8(8)	H12 -C12 -C11	119.5
C3 -C2 -C1	120.4(8)	H12 -C12 -C13	120.1
C7 -C2 -C1	119.1(8)	Rh -N2 -HN2	121.9
C7 -C2 -C3	120.5(8)	HN2 -N2 -C14	122.0
C4 -C3 -C2	119.7(9)	H15A -C15 -C16	108.1
C5 -C4 -C3	120.0(10)	H15B -C15 -C16	108.0
C6 -C5 -C4	120.4(10)	H15B -C15 -H15A	110.0
C7 -C6 -C5	122.0(10)	H16A -C16 -C15	110.4
C6 -C7 -C2	117.4(9)	H16B -C16 -C15	110.2
C8 -C7 -C2	120.5(8)	H16B -C16 -H16A	109.8
C8 -C7 -C6	122.1(9)	H17A -C17 -C18	110.3
C9 -C8 -C7	120.5(9)	H17B -C17 -C18	109.9
C13 -C8 -C7	121.8(8)	H17B -C17 -H17A	109.7

Table S16 continued.

	Angle(°)
H18A –C18 –C17	107.9
H18B –C18 –C17	108.0
H18B –C18 –H18A	109.4
H19A –C19 –C20	108.9
H19B –C19 –C20	109.0
H19B –C19 –H19A	109.6
H20A –C20 –C19	110.2
H20B –C20 –C19	110.1
H20B –C20 –H20A	110.0
H21A –C21 –C22	110.0
H21B –C21 –C22	109.9
H21B –C21 –H21A	109.9
H22A –C22 –C21	108.1
H22B –C22 –C21	108.6
H22B –C22 –H22A	109.7

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Table S15. Distances Less Than 3.5 Å of [Rh([12]aneS4)phi]Br3 x 3H2O

	Distance(Å)		Distance(Å)
N1 -Br3	3.308(7)	C21 -H11	3.050
C4 -C11	3.270(15)	C21 -H12	3.230
C6 -W3	3.494(13)	C22 -H11	2.918
C10 -W2	3.384(13)	C22 -H12	3.470
C11 -W2	3.464(13)	Br1 -H16B	3.035
C14 -W1	3.310(12)	Br1 -H22B	2.751
N2 -W1	3.125(10)	Br1 -H11	3.285
C16 -W2	3.281(12)	Br1 -H19B	3.410
S3 -W1	3.309(8)	Br1 -H20B	2.971
C19 -W1	3.427(12)	Br1 -H16A	3.414
C22 -Br3	3.475(10)	Br1 -H17A	3.031
Br1 -W2	3.389(8)	Br2 -H18B	2.899
Br1 -W3	3.301(8)	Br2 -H19A	3.009
Br1 -W2	3.319(8)	Br2 -HN1	2.815
Br2 -W3	3.348(8)	Br2 -H3	2.932
Br2 -W1	3.344(7)	Br2 -H18A	2.874
W1 -W3	2.837(11)	Br3 -H21A	3.080
C2 -H22A	3.055	Br3 -H22A	2.836
C3 -H22A	3.070	Br3 -H12	3.077
C4 -H11	2.978	Br3 -HN2	2.977
C4 -H4	3.090	Br3 -H20A	2.922
C4 -H5	3.335	Br3 -H21A	2.853
C4 -H22A	3.492	Br3 -HN1	2.748
C5 -H11	3.059	Br3 -H3	3.246
C5 -H4	3.033	Br3 -H15A	2.915
C7 -H15B	3.231	W1 -H12	3.412
C8 -H15B	2.819	W1 -HN2	3.035
C9 -H18B	3.459	W1 -H19A	3.056
C9 -H15B	3.186	W1 -H20A	2.902
C10 -H4	3.455	W1 -H3	3.000
C11 -H4	3.036	W1 -H4	2.982
C11 -H5	3.472	W1 -H5	2.644
C11 -H21B	2.789	W2 -H20B	3.472
C11 -H22A	3.303	W2 -H21B	2.851
C12 -H4	3.156	W2 -H15A	3.201
C12 -H21B	3.013	W2 -H15B	3.498
C12 -H22A	3.419	W2 -H16A	2.457
C13 -H15A	3.434	W2 -H10	3.326
C13 -H15B	3.079	W2 -H11	3.481
C16 -H16A	3.278	W2 -H17B	2.700

Table S17 continued.

		Distance(Å)
W3	-H5	3.198
W3	-H6	2.820
W3	-H19A	3.480
W3	-H17A	3.130
W3	-H18A	2.856
H3	-H12	3.479
H3	-H22A	3.329
H4	-H11	3.030
H4	-H12	3.259
H4	-H4	2.526
H4	-H5	2.402
H5	-H10	3.467
H5	-H11	3.128
H9	-H17A	3.046
H9	-H18B	2.811
H10	-H17B	3.384
H10	-H18B	2.935
H10	-H19B	2.881
H11	-H21B	2.410
H11	-H22A	2.607
H11	-H22B	2.710
H12	-H21A	3.083
H12	-H21B	2.803
H12	-H22A	2.842
H15A	-H21B	3.493
H16A	-H16A	2.955
H16A	-H16B	2.821
H16A	-H17A	3.315
H16A	-H17B	3.081
H16B	-H16B	3.463
H16B	-H17A	3.471
H18A	-H18A	3.376

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Table S16. Distances of Atoms of Ancillary Ligands NH_3, en2[a], [12]aneN4 and [12]aneS4 of Complexes $[Rh(X)_4phi]^{3+}$ to Planes A, B and C[b].

atom	ligand X	a-value	b-value	c-value
X1	NH_3	2.068	-0.013	0.062
	en2	2.027	0.040	0.085
	N4	2.027	-0.081	0.401
	S4	2.357	0.117	0.253
C2	en2	2.481	0.804	1.265
	N4	2.398	1.097	1.260
	S4	2.568	1.671	1.245
C3	en2	1.572	2.009	1.481
	N4 (C_s)	1.343	2.096	1.331
	N4 (C_{2v})	1.308	1.525	2.230
	S4	1.383	2.577	1.163
X4	NH_3	-0.050	1.473	1.471
	en2	0.164	1.451	1.460
	N4	0.053	1.473	1.390
	S4	-0.079	1.613	1.641
C5	N4 (C_s)	-1.134	2.250	1.235
	N4 (C_{2v})	-1.247	1.693	2.204
	S4	-1.552	2.504	1.090
C6	N4	-2.325	1.363	1.151
	S4	-2.695	1.513	1.158
X7	NH_3	-2.061	0.001	-0.044
	en2	-2.064	-0.058	0.056
	N4	-2.039	0.120	0.323
	S4	-2.346	-0.024	0.210
C8	en2	-2.452	-1.321	0.676
	N4	-2.423	-1.135	1.054
	S4	-2.590	-1.271	1.507
C9	en2	-1.630	-1.619	1.817
	N4	-1.344	-1.511	2.034
	S4	-1.429	-1.407	2.484
X10	NH_3	-0.017	-1.454	1.481
	en2	-0.161	-1.458	1.443
	N4	-0.081	-1.543	1.303
	S4	+0.034	-1.735	1.497
C11	N4	1.197	-1.679	2.053
	S4	1.477	-1.307	2.522
C12	N4	2.302	-1.390	1.077
	S4	2.617	-1.151	1.562

[a]Distances are given for the Λ-enantiomer. [b]A schematic structure with the numbering scheme is shown in Figure 2.

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Table S2. UV-Visible Data of Phi Complexes of Rhodium(III) at Different pH.

complex	pK_a[a]	pH	λ_{max} [nm](ε x 10^{-3}[$M^{-1}cm^{-1}$])[b]
$[Rh(NH_3)_4phi]^{3+}$	9.2	pH 11	255 (22.2), 264 (25.2), 273 (24.8), 283 (sh, 13.4), 364 (sh, 8.0), 373 (8.1)
		pH 7[d]	252 (16.3), 263 (sh, 20.5), 270 (24.6), 283 (sh, 10.5), 372 (11.7), 386 (sh, 10.4)
			isosb. points: 268 (23.5), 333 (4.2)
$[Rh(en)_2phi]^{3+}$	9.1	pH 11	254 (23.6), 264 (26.2), 273 (25.7), 283 (14.2), 363 - 375 (broad, 9.2)
		pH 7[d]	252 (17.9), 263 (sh, 21.9), 271 (25.6), 283 (11.6), 376 (13.4), 389 (sh, 12.3)
			isosb. points: 269 (24.2), 336 (5.1)
$[Rh([12]aneN_4)phi]^{3+}$[c]	9.0	pH 11	252 (35.7), 264 (31.1), 272 (28.8), 287 (sh, 15.2), 384 (12.1)
		pH 7[d]	252 (27.3), 263 (26.6), 271 (28.8), 287 (sh, 12.9), 395 (16.7), 410 (sh, 15.2)
			isosb. point: 359 (9.1)
$[Rh([12]aneS_4)phi]^{3+}$	4.7	pH 7[e]	252 (30.8), 261 (sh, 35.5), 268 (39.3), 283 (sh, 20.8), 331 (sh, 11.4), 359 (15.3)
		pH 2	252 (27.6), 265 (27.9), 288 (15.3), 381 (17.6)
			isosb. points: 288 (15.3), 306 (7.0), 364 (15.0)

[a]Optical pK_a-values, for comparison: pK_a of $[Rh(phen)_2phi]^{3+}$ is 6.2. [b]Spectra were recorded in water, pH was adjusted by adding either dilute HCl or NaOH. [c]Mixture of two isomers (60:40). [d]The spectra at lower pH are identical. [e]The spectra at higher pH (up to pH 10) are identical. [e]Irreversible decomposition occurs above pH 10.

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Figure S1. (A) ORTEP drawing of the contents of a unit cell of [Rh([12]aneN$_4$)phi](SCN)$_3$ x 2H$_2$O, with a unit cell outlined. Atoms are are shown as 50 % probability ellipsoids. Hydrogen atoms on N(3), N(4), N(5) and N(6) are shown with thermal parameters 10 % of those assigned. The rhodium atom is shown with shaded octant, the sulfur atoms and the water oxygen atoms with outlined octants. The view is perpendicular to the a b plane. Only the major components of the disordered atoms are shown. (B) View perpendicular to two phenanthrenequinone diimine ligands indicating partial overlap of the π-systems.

Figure S2. (A) ORTEP drawing of the contents of a unit cell of [Rh([12]aneS$_4$)phi]Br$_3$ x 3H$_2$O, with a unit cell outlined. Atoms are are shown as 50 % probability ellipsoids. Hydrogen atoms are not shown. The rhodium and bromide atoms are shown with shaded octants, the water oxygen atoms with outlined octants. The view is perpendicular to the b c plane. (B) View perpendicular to two phenanthrenequinone diimine ligands indicating partial overlap of the π-systems.

Figure S3. Proton decoupled ^{13}C NMR spectrum (D$_2$O, 75.47 MHz) of a mixture of the two isomers of [Rh([12]aneN$_4$)phi]$^{3+}$ in thermodynamic equilibrium (an asterisk denotes resonances assigned to the isomer of point group C$_{2v}$). The inset shows an HPL-chromatogram of a mixture of the two isomers (chromatographic conditions see Experimental Section).

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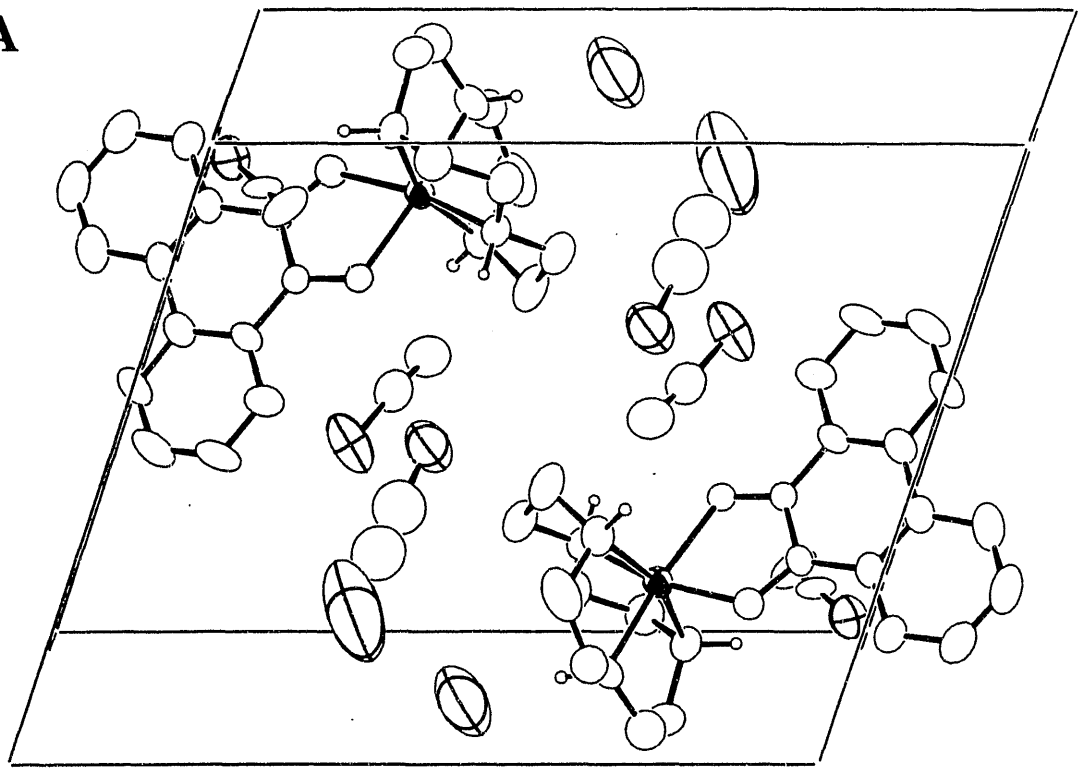
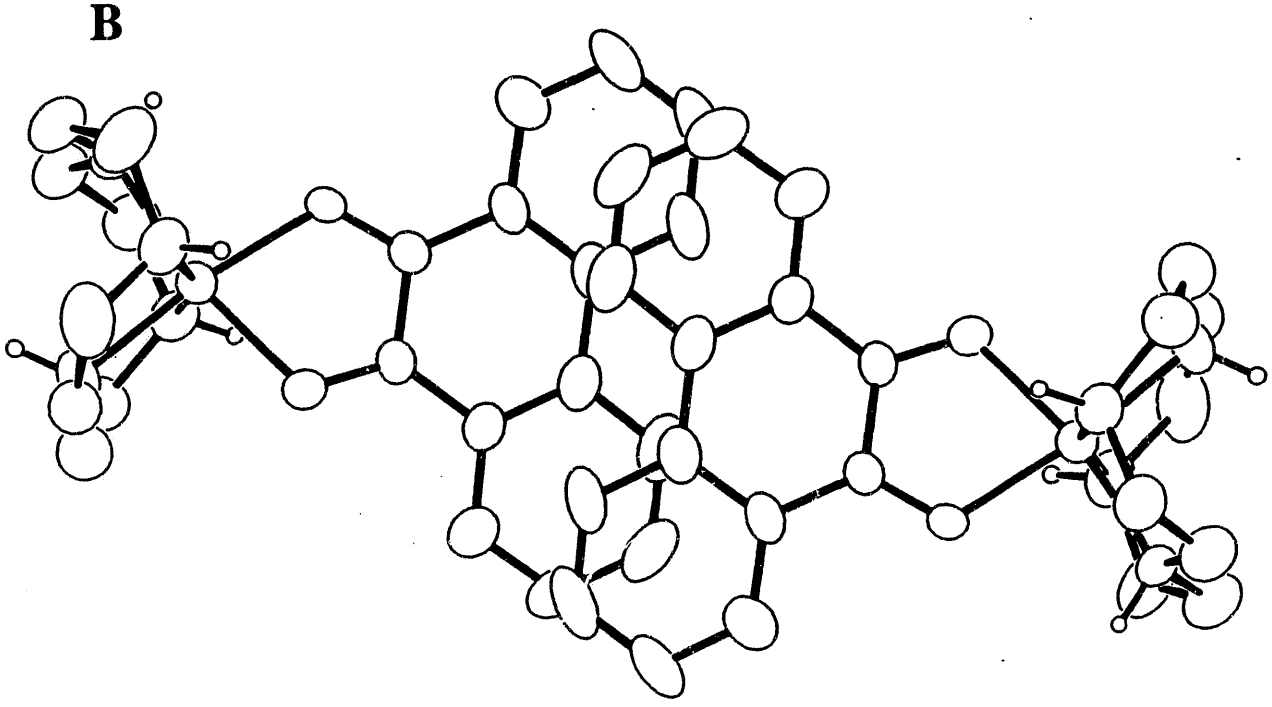
A

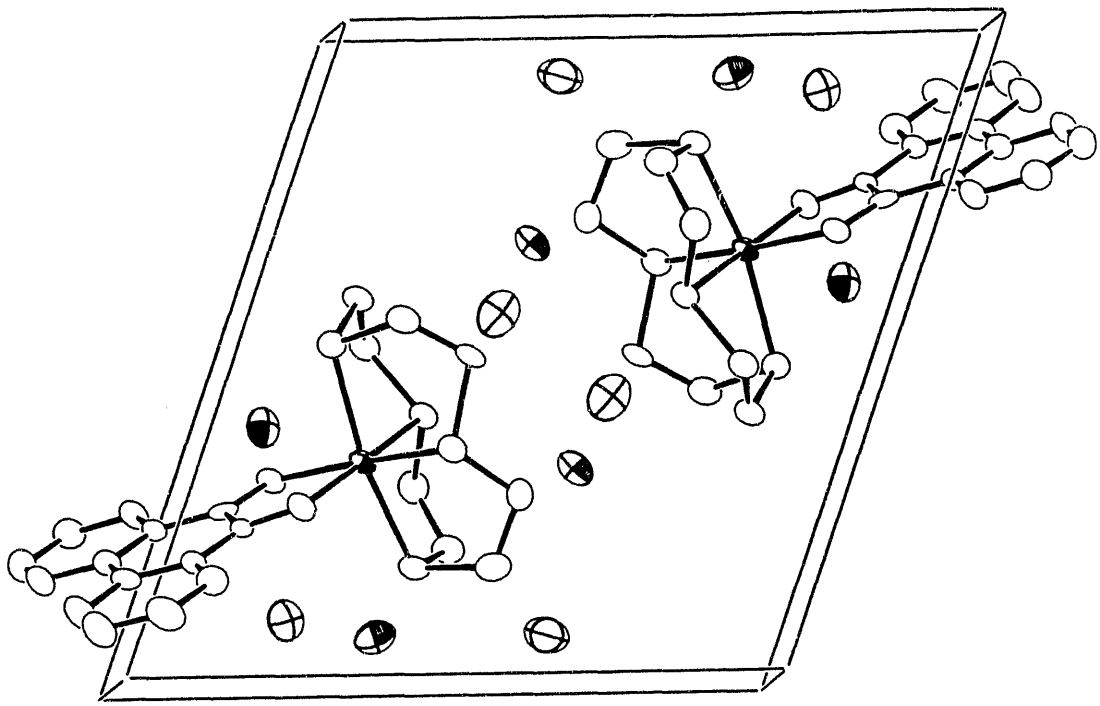


B



Suppl. Mat. "Metallointercalators: Syntheses...." Krotz, A. H. et al.

A



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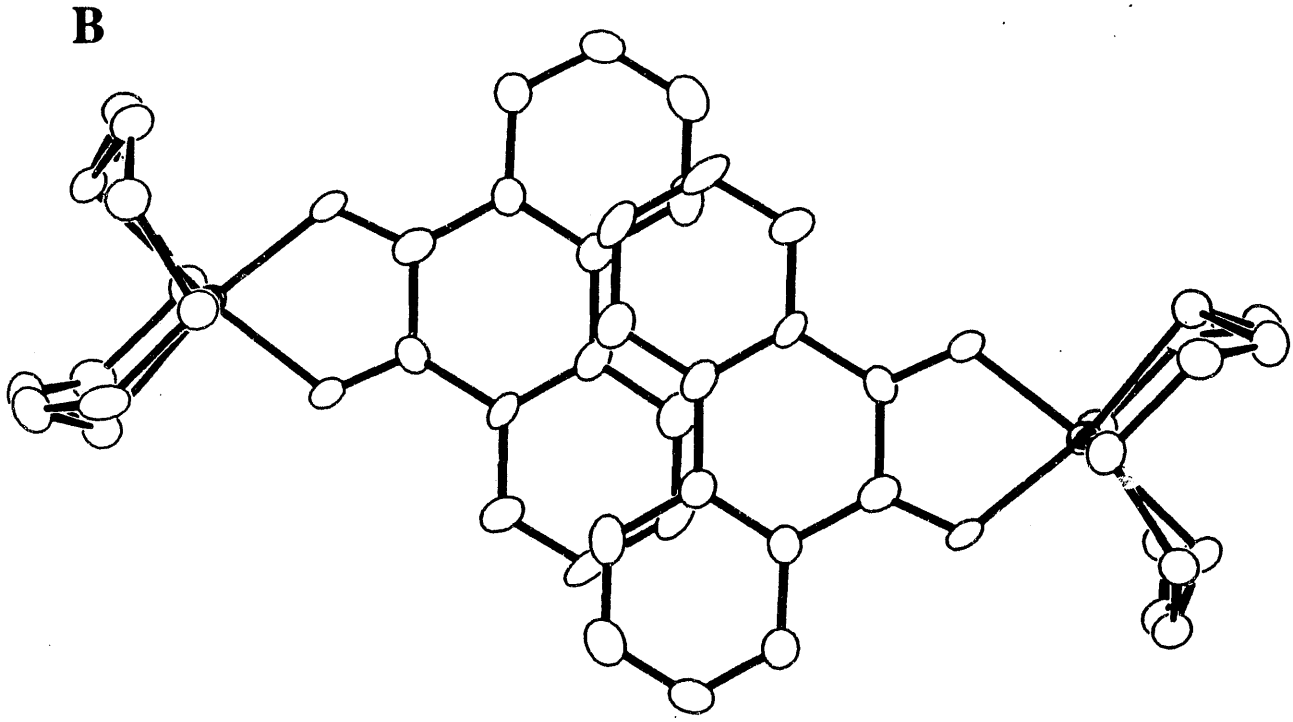

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